Module 5

Simple Linear Regression and Calibration

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Calibration of a Measurement Device

Calibration is an essential activity in the qualification and maintenance of measurement devices or systems. The basic idea is to use a measurement device to produce measurements on "standard" specimens with (relatively well-) "known" values of measurands, and see how the measurements compare to the measurands. In the event that there are systematic discrepancies between what is known to be true and what the device reads (in the event that there are device biases), the plan is then to invent some conversion scheme to (in future use of the device) adjust what is read to remove the biases. A slight extension of "regression" analysis (curve fitting) from an elementary statistics course is the relevant statistical methodology in making this conversion.

Simple Linear Regression

Calibration studies employ true/gold-standard-measurement values of measurands x and "local" measurements y. (Strictly speaking, y need not even be in the same units as x.) Regression analysis can provide both "point conversions" and measures of uncertainty (the latter through inversion of "prediction limits"). The simplest version of this is where observed measurements are approximately linearly related to measurands, i.e.

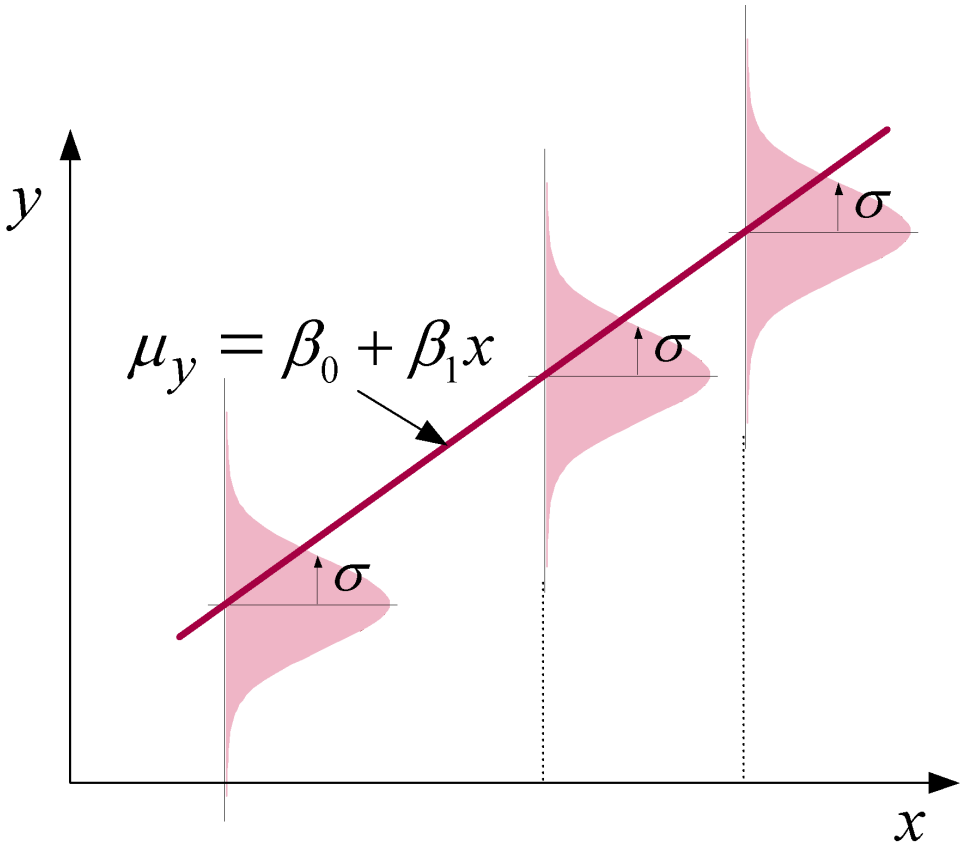
$$y \approx \beta_0 + \beta_1 x$$

This is "linear calibration." The standard statistical model for such a circumstance is

$$y = \beta_0 + \beta_1 x + \epsilon \quad .$$

Simple Linear Regression (cont.)

The SLR model is typically pictured as below.



Simple Linear Regression (cont.)

For n data pairs (x_i, y_i), simple linear regression methodology allows one to make confidence intervals and tests associated with the model, and *prediction limits for a new measurement* y_{new} *associated with a new measurand*, x_{new}. These are of the form

$$(b_0 + b_1 x_{\text{new}}) \pm t s_{\text{LF}} \sqrt{1 + \frac{1}{n} + \frac{(x_{\text{new}} - \bar{x})^2}{\sum_i (x_i - \bar{x})^2}}$$

where the least squares line is $\hat{y} = b_0 + b_1 x$ and s_{LF} (a "line-fitting" sample standard deviation) is an estimate of σ derived from the fit of the line to the data. Any good statistical package will compute and plot these limits as functions of x_{new} along with a least squares line through the data set.

The Relevance of SLR to Calibration Problems

What is here of most interest about simple linear regression technology is what it says about calibration and measurement in general. Some applications of inference methods based on the SLR model to metrology are the following.

- From a simple linear regression output,

$$s_{\mathrm{LF}} = \sqrt{MSE} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}\left(y_i - \hat{y}_i\right)^2} = \text{"root mean square error"}$$

  is an estimated repeatability standard deviation. One may make confidence intervals for $\sigma = \sigma_{\text{repeatability}}$ based on the estimate using $\nu = n - 2$ degrees of freedom and limits

$$s_{\mathrm{LF}}\sqrt{\frac{n-2}{\chi^2_{\text{upper}}}} \qquad \text{and} \qquad s_{\mathrm{LF}}\sqrt{\frac{n-2}{\chi^2_{\text{lower}}}}.$$

The Relevance of SLR to Calibration Problems (cont.)

- The least squares equation $\hat{y} = b_0 + b_1 x$ can be solved for x, giving

$$\hat{x}_{\text{new}} = \frac{y_{\text{new}} - b_0}{b_1}$$

  as a way of estimating a new "gold-standard" value (a new measurand, x_{new}) from a measured local value, y_{new}. If the relationship between measurand and average measurement is a straight line relationship, this should at least approximately remove bias in measurement.

- One can take prediction limits for y_{new} and "turn them around" to get confidence limits for the x_{new} corresponding to a measured local y_{new}. This provides a defensible way to set "error bounds" on what y_{new} indicates about x_{new}.

The Relevance of SLR to Calibration Problems (cont.)

- In cases where y and x are in the same units, confidence limits for the slope β_1 of the simple linear regression model

$$b_1 \pm t \frac{s_{\mathrm{LF}}}{\sqrt{\sum (x_i - \bar{x})^2}}$$

provide a way of investigating the constancy of bias (linearity of the measurement device in the sense used thus far today). That is, when x and y are in the same units, $\beta_1 = 1.0$ is the case of constant bias. If confidence limits for β_1 fail to include 1.0, there is clear evidence of device nonlinearity.

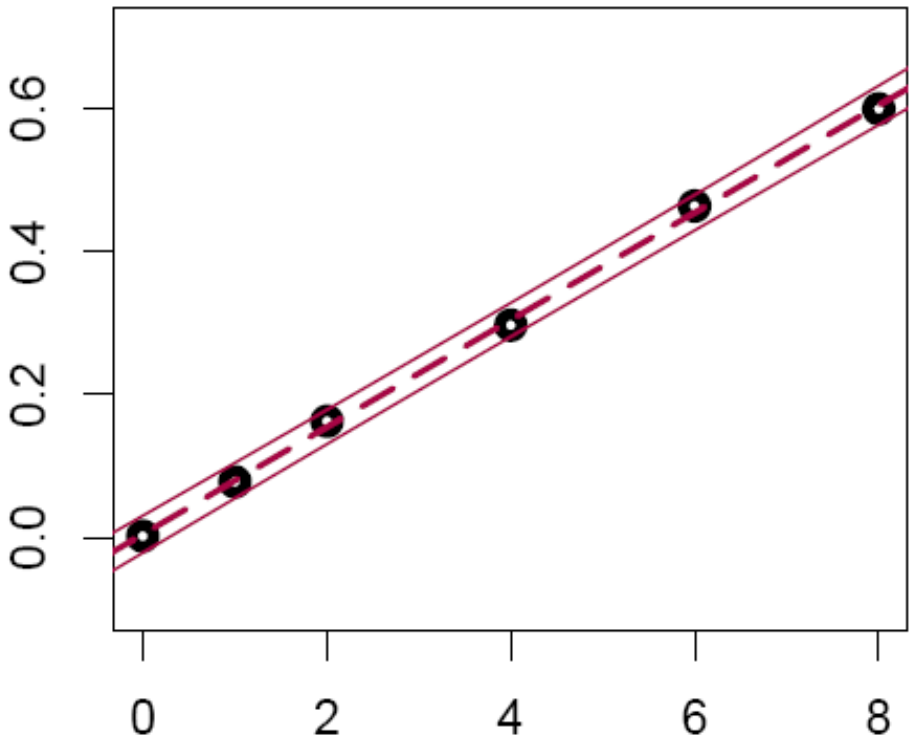
Example 5-1

Measuring Cr^{6+} Concentration With a UV-vis Spectrophotometer. The data below were taken from a Web page of the School of Chemistry at the University of Witwatersrand developed and maintained by Dr. Dan Billing. They are measured absorbance values, y, for $n = 6$ solutions with "known" Cr^{6+} concentrations, x (in $\mathrm{mg/l}$), from an analytical lab.

x	0	1	2	4	6	8
y	.002	.078	.163	.297	.464	.600

Example 5-1 (cont.)

A plot of these data, the corresponding least squares line, and 95% prediction limits for y_{new} at each x_{new} between 0 and 8.0 is below.



Example 5-1 (cont.)

Use of the ™JMP statistical package produces

$$y = .0048702 + .0749895x \quad \text{with } s_{\text{LF}} = .007855 \ .$$

We might expect a local (y) repeatability standard deviation of around .008 (in the y absorbance units). In fact, 95% confidence limits for σ can be made (using $n - 2 = 4$ degrees of freedom) as

$$.007855\sqrt{\frac{4}{11.143}} \quad \text{and} \quad .007855\sqrt{\frac{4}{.484}} \ ,$$

i.e.

$$.0047 \quad \text{and} \quad .0226 \ .$$

Making use of the slope and intercept of the least squares line, a conversion formula for going from y_{new} to x_{new} is

$$\hat{x}_{\text{new}} = \frac{y_{\text{new}} - .0048702}{.0749895} \ .$$

Example 5-1 (cont.)

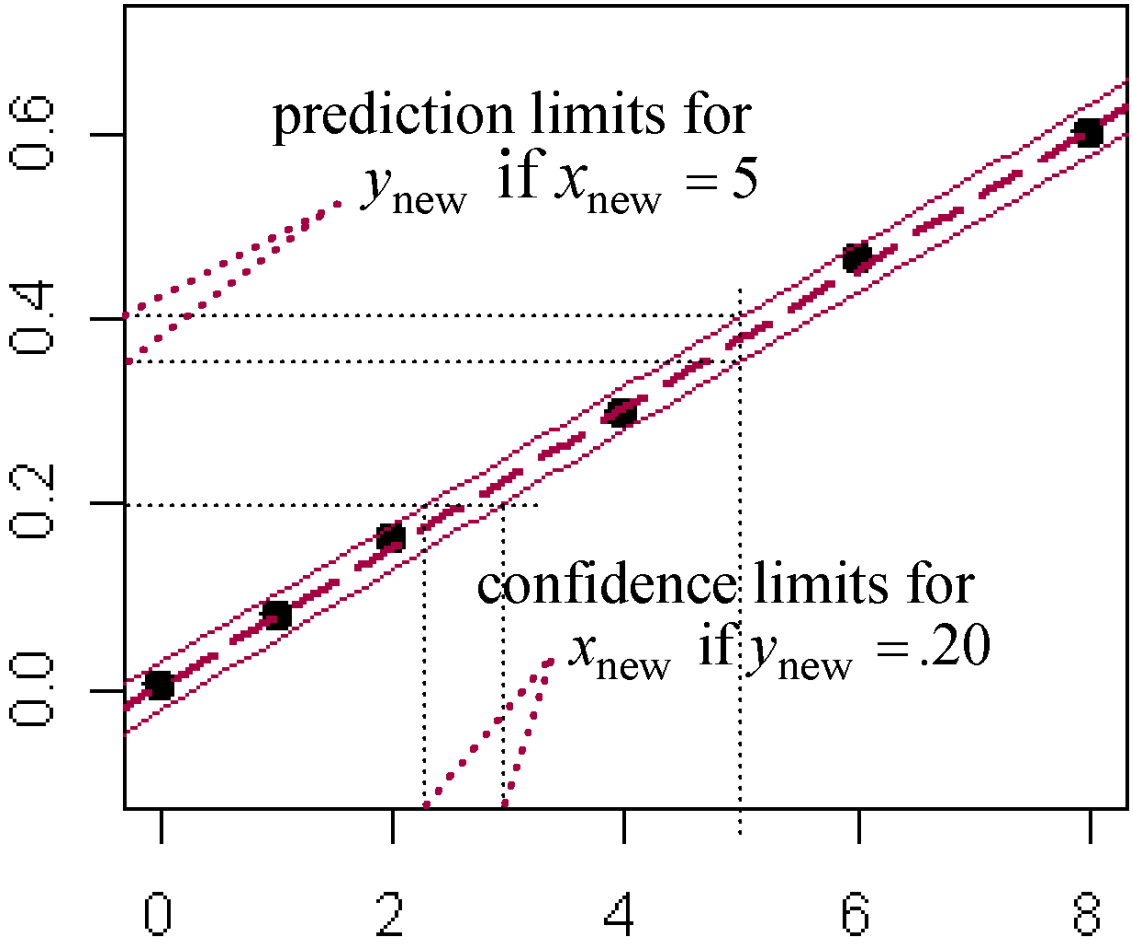
So, for example, a future measured absorbance of $y_{\text{new}} = .20$ suggests a concentration of

$$\hat{x}_{\text{new}} = \frac{.20 - .0048702}{.0749895} = 2.60\,\mathrm{mg}/\mathrm{l}\ .$$

Finally, the figure on the next panel illustrates how prediction limits provide both 95% predictions for a new measurement on a fixed/known measurand *and* 95% confidence limits on a new measurand, having observed a particular measurement. Reading from the figure, one is "95% sure" that a future observed absorbance of .20 comes from a concentration between

$$2.28\,\mathrm{mg}/\mathrm{l} \ \text{ and } \ 2.903\,\mathrm{mg}/\mathrm{l}\ .$$

Example 5-1 (cont.)



Example 5-2

A Check on Device "Linearity." A calibration data set due to John Mandel compared $n = 14$ measured values y for a single laboratory to corresponding consensus values x for the same specimens derived from multiple labs. (The units are not available, but were the same for x and y values.) A simple linear regression analysis of the data pairs produced

$$b_1 = .882 \quad \text{and} \quad \frac{s_{\text{LF}}}{\sqrt{\sum (x_i - \bar{x})^2}} = .012$$

so that (using the upper 2.5% point of the t_{12} distribution, 2.179) 95% confidence limits for β_1 are

$$.882 \pm 2.179\,(.012)$$

or

$$.882 \pm .026\ .$$

A 95% confidence interval for β_1 clearly does not include 1.0. So bias for the single laboratory was not constant. (The measurement "device" was not linear in the sense we have used the word here.)